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A New Class of Efficient SAV Schemes with Lagrange Multipliers for Dissipative Systems with Global Constraints

Yanrong Zhang[1,2] and Jie Shen[1,3,*]

[1]*School of Mathematical Sciences and Fujian Provincial Key Laboratory on Mathematical Modeling and High Performance Scientific Computing, Xiamen University, Xiamen, Fujian, 361005, China.*
[2]*Department of Applied Mathematics, The Hong Kong Polytechnic University, Hung Hom, Hong Kong SAR, China.*
[3]*Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA.*

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Dedicated to Professor Tao Tang on occasion of his 60th birthday.

Abstract. In this paper, we develop a class of efficient and accurate numerical schemes for general dissipative systems with global constraints. The schemes are based on the relaxed generalized SAV approach and the Lagrange multiplier approach, and enjoy many advantages such as solving only one linear system with constant coefficients and one nonlinear algebraic system for the Lagrange multipliers. Besides, the schemes preserve global constraints and are unconditionally energy stable with a modified energy, which is equal to the original energy in most cases. We present applications of the R-GSAV/LM approach to a variety of problems to demonstrate its effectiveness and advantages compared with existing approaches.

AMS subject classifications: 35Q40, 65M12, 35Q55, 65M70
Key words: SAV, dissipative system with global constraints, Lagrange multiplier, stability.

1. Introduction

Solutions for a large class of partial differential equations (PDEs) arising in physical, chemical, and biological sciences are not only energy dissipative, but also satisfy certain global constraints, such as preservation of norm, volume, surface area, etc. It is important to develop numerical schemes, which are energy dissipative and preserve these constraints at the discrete level.

While there are many different ways to design numerical schemes that are energy dissipative — cf. [11,13,19–23,26,27], there are relatively few approaches to preserve global constraints, among which the two popular ones are:

*Corresponding author. *Email addresses:* yanrongzhang_math@163.com (Y. Zhang), shen7@purdue.edu (J. Shen)

- **The penalty approach**. This approach is frequently used to deal with gradient flows with global constraints (cf. [7,16,18,24,27,30]). The key is to add suitable penalty terms related to global constraints in the free energy of the underlying gradient flow. Then, one can apply usual methods for the new gradient flow with the augmented free energy. The drawback of this approach is that the problem may become very stiff as we increase the penalty strength to better preserve the constraints.

- **The Lagrange multiplier approach**. The main idea is to introduce Lagrange multipliers to enforce the global constraints (cf. [6,12]). Although the Lagrange multiplier approach can in principle preserve the global constraints exactly, how to develop efficient, robust and energy stable numerical schemes for the system with Lagrange multipliers is still challenging. In [8], the authors proposed three numerical schemes for the Lagrange multiplier approach with different advantages and shortcomings. A particular issue is that the Lagrange multipliers are determined by solving a nonlinear algebraic system which may require exceedingly small time steps to have a suitable solution. This approach is also applied to nonlinear Schrödinger/Gross-Pitaevskii equations in [1] and Klein-Gordon Schrödinger (KGS) equations in [28]. It is found in [1] that, in some situations, the nonlinear algebraic system for the Lagrange multipliers may not admit a solution even at very small time steps.

In this paper, we propose a class of new schemes, referred hereafter to as the relaxed generalized SAV/Lagrange multiplier (R-GSAV/LM) approach, for general dissipative complex nonlinear systems with global constraints. This class of schemes combines the ideas and advantages of the relaxed generalized SAV (R-GSAV) approach [15,17,29] and the Lagrange multiplier approach [8]. More precisely, (i) the generalized SAV approach [15] is used to ensure unconditional stability with a modified energy; (ii) the Lagrange multiplier approach [8] is used to enforce the global constraints; and (iii) the relaxation idea in [17,29] is used to improve the accuracy by relating the modified energy to the true energy. This class of schemes enjoys the following advantages: (i) it only requires solving one linear system with constant coefficients so it is very efficient; (ii) it can be higher-order accurate; (iii) it can preserve global constraints exactly by solving a nonlinear algebraic system for the Lagrange multipliers only, so it is much more robust as the Lagrange multipliers are decoupled from the SAV; (iv) it is unconditionally energy stable with a modified energy which, in most cases, equals to the original energy.

We apply our new schemes to several interesting models, including single-component and multi-component Bose Einstein Condensates (BECs), an optimal partition problem with multiple constraints, and Klein-Gordon-Schrödinger (KGS) equations.

The rest of this paper is organized as follows. In Section 2, we briefly review the Lagrange multiplier approaches in [8], and for the purpose of comparison, extend the second approaches in [8] to higher-order. In Section 3, we introduce our R-GSAV/LM approach for general dissipative systems, and derive a stability result. In Section 4, we apply our new schemes to imaginary time gradient flow of one- and multi-component BECs, optimal partition problem with multiple constraints, and KGS equations. Some concluding remarks are presented in Section 5.